

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
19 May 2005 (19.05.2005)

PCT

(10) International Publication Number
WO 2005/045726 A3

(51) International Patent Classification⁷: **G01N 23/207**

(21) International Application Number:
PCT/US2004/035444

(22) International Filing Date: 27 October 2004 (27.10.2004)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/514,523 27 October 2003 (27.10.2003) US
60/546,976 24 February 2004 (24.02.2004) US

(71) Applicant (for all designated States except US): SSCI,
INC. [US/US]; 3065 Kent Avenue, W. Lafayette, Indiana
47906 (US).

(72) Inventors; and

(75) Inventors/Applicants (for US only): BATES, Simon

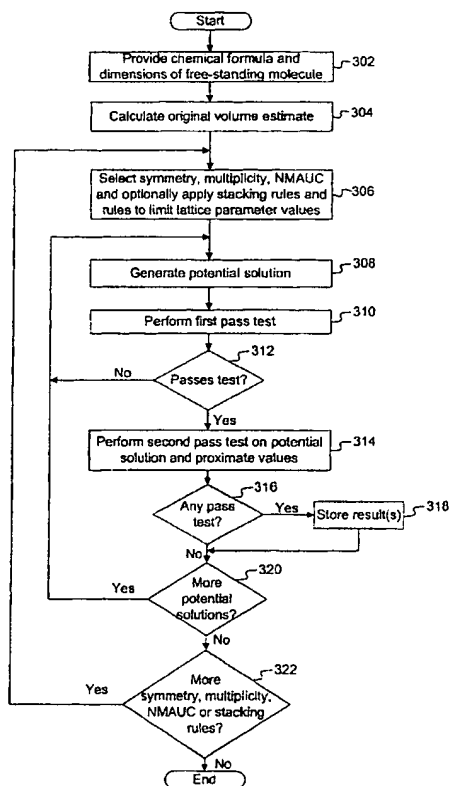
[US/US]; 3343 Peppermill Drive, West Lafayette, Indiana
47906 (US). IVANISEVIC, Igor [US/US]; 331 Secretariat
Circle, West Lafayette, IN 47906 (US). STAHLY, Bar-
bara C. [US/US]; 3908 Sunnycroft Place, West Lafayette,
Indiana 47906 (US).

(74) Agents: GARRETT, Arthur S. et al.; Finnegan, Hender-
son, Farabow Garrett & Dunner, LLP, 901 New York Av-
enue, NW, Washington, D.C. 20001-4413 (US).

(81) Designated States (unless otherwise indicated, for every
kind of national protection available): AE, AG, AL, AM,
AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI,
GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE,
KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG,
PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM,
ZW.

[Continued on next page]

(54) Title: METHOD FOR MONTE CARLO INDEXING OF POWDER DIFFRACTION DATA



(57) Abstract: Crystalline solid forms may be characterized by their unit cell parameters through a process known as indexing. An embodiment of the invention searches for the unit cell parameters of a crystalline solid form using a Monte-Carlo algorithm that incorporates certain rules to reduce search space. Another embodiment refines the results of the search to identify the correct unit cell parameters of the crystalline solid form. These methods may be automated, conveniently requiring little interaction from the user. The indexing method of the invention may be applied, for example, to distinguish between different crystalline solid forms of a substance.

WO 2005/045726 A3



(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

— with international search report

— before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments

(88) Date of publication of the international search report:

6 October 2005

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.